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Monte Carlo path-integral methods for vibrational-rotational partition functions

Author: Lynch, Vanessa Marie Audette

Degree: Ph.D.

Year: 2005

Corporate Source/Institution: University of Minnesota (0130) Source: VOLUME 66/03-B OF DISSERTATION ABSTRACTS INTERNATIONAL.

PAGE 1490. 214 PAGES

ISBN:

0-542-03589-8

...super>OOH, and H<super>18</super>OOD). The path centroids are sampled in Jacobi coordinates via a set of independent ziggurat schemes. The calculations employ enhanced-same- path extrapolation of trapezoidal Trotter Fourier path integrals, which are constructed using fast Fourier sine transforms. Importance...

...a more extensive look at their use in statistical mechanics. This chapter also explores various path integral statistical mechanical methods for determining partition functions. Chapter 2 presents the first work on calculating an accurate vibrational-rotational partition...

Ginger R. DeMille

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